Isophorone

78-59-1 | DTXSID8020759

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 2.28

Global applicability domain: Inside

Local applicability domain index: 7.31e-01

Confidence level: 6.27e-01

Nearest Neighbors from the Training Set

Image not found
Isophorone
Measured: 1.70
Predicted: 2.28

Image not found
Carveol
Measured: 3.12
Predicted: 2.91

Image not found
Piperitone
Measured: 2.85
Predicted: 2.82

Image not found
4-Isopropenylcyclohex-1-en-1-ylmethanol
Measured: 3.17
Predicted: 2.95